

Sum rules, dipole oscillation and spin polarizability of a spin-orbit coupled quantum gas

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Abstract – Using a sum rule approach we investigate the dipole oscillation of a spin-orbit coupled Bose-Einstein condensate confined in a harmonic trap. The crucial role played by the spin polarizability of the gas is pointed out. We show that the lowest dipole frequency exhibits a characteristic jump at the transition between the stripe and spin-polarized phase. Near the second order transition between the spin-polarized and the single minimum phase the lowest frequency is vanishingly small for large condensates, reflecting the divergent behavior of the spin polarizability. We compare our results with recent experimental measurements as well as with the predictions of effective mass approximation.

Synthetic gauge fields represent a rapidly developing direction of research in ultra cold atomic physics both from the experimental [1–10] and theoretical perspective [11–26]. They give rise to the occurrence of new quantum phases exhibiting unique magnetic features. In the presence of spin-orbit coupling also the collective oscillations exhibit challenging features which have been already the object of theoretical studies [27–31], as well as first experimental measurements [8]. In particular the experiment of [8] has shown that the center-of-mass oscillation of a harmonically trapped Bose-Einstein condensate can be deeply affected by the coupling with the spin degree of freedom. In the same paper the problem was investigated theoretically using a variational approach within time dependent Gross-Pitaevskii theory.

The purpose of the present work is to study the behavior of the center-of-mass oscillation employing a sum rule approach. This method is known to point out the role of conservation laws and to reduce the calculation of the dynamical properties of the many-body system to the knowledge of a few key parameters relative to the ground state. In the case of the center-of-mass oscillation we will show that, due to the spin-orbit coupling, a key role is played by the spin polarizability of the gas which is responsible for important deviations of the dipole frequency from the harmonic oscillator value.

In this work we consider a spin 1/2 interacting gas characterized by the Hamiltonian (for simplicity we set

$\hbar = m = 1$)

$$H = \sum_i h_0(i) + \sum_{\alpha, \beta} \frac{1}{2} \int d^3\mathbf{r} g_{\alpha\beta} n_{\alpha}(\mathbf{r}) n_{\beta}(\mathbf{r}) \quad (1)$$

where $i = 1, \dots, N$ is the particle index, while α and β are the spin indices ($\uparrow, \downarrow = \pm$) characterizing the two spin states. The single-particle Hamiltonian h_0 is defined by

$$h_0 = \frac{1}{2} [(p_x - k_0 \sigma_z)^2 + p_{\perp}^2] + \frac{\Omega}{2} \sigma_x + \frac{\delta}{2} \sigma_z + V_{\text{ext}}(\mathbf{r}) \quad (2)$$

and is characterized by equal contributions of Rashba [32] and Dresselhaus [33] spin-orbit couplings and a uniform magnetic field in the (x, z) -plane, with Ω the Raman coupling constant accounting for the transition between the two spin states, k_0 the momentum transfer of the two Raman lasers, δ the energy difference between the two single-particle spin states, and $V_{\text{ext}} = (\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2)/2$ the external trapping potential, thereby chosen of harmonic type. The spin up and down density operators entering Eq. (1) are defined by $n_{\pm}(\mathbf{r}) = (1/2) \sum_i (1 \pm \sigma_{z,i}) \delta(\mathbf{r} - \mathbf{r}_i)$ while $g_{\alpha\beta} = 4\pi a_{\alpha\beta}$ are the relevant coupling constants in the different spin channels, with $a_{\alpha\beta}$ the corresponding s -wave scattering lengths. Finally σ_k , with $k = x, y, z$, are the usual 2×2 Pauli matrices. The Hamiltonian (1), (2) has been already implemented experimentally [4, 8]. It has been recently employed to describe a variety of non trivial quantum phases in Bose-Einstein condensates [18, 19].

In the absence of spin-orbit coupling ($k_0 = 0$) the center-of-mass oscillation of the trapped gas along the x -direction is exactly excited by the operator $X = \sum_i x_i$ and corresponds to the usual sloshing mode with frequency ω_x . In order to investigate the effect of spin-orbit coupling it is useful to introduce the following moments of the excitation strengths of the operator F at zero temperature¹:

$$m_k(F) = \sum_n (E_n - E_0)^k |\langle 0|F|n\rangle|^2 \quad (3)$$

where $|0\rangle$ and $|n\rangle$ are, respectively, the ground state and the excited states of H with $E_n - E_0$ the corresponding excitation energies, while $|\langle 0|F|n\rangle|^2$ is the F -strength relative to the state $|n\rangle$. Some relevant sum rules can be easily calculated employing the closure relation and the commutation rules involving the Hamiltonian of the system. For example the most famous energy-weighted moment for the dipole operator $F = X$ takes the model independent value (also called f -sum rule) $m_1(X) = (1/2)\langle 0|[X, [H, X]]|0\rangle = N/2$ where N is the total number of atoms. Notice that this sum rule is not affected by the spin terms in the Hamiltonian, despite the fact that the commutator of H with X explicitly depends on the spin-orbit coupling:

$$[H, X] = -i(P_x - k_0 \Sigma_z). \quad (4)$$

Here $P_x = \sum_i p_{x,i}$ is the total momentum of the gas along x and $\Sigma_z = \sum_i \sigma_{z,i}$ is the total spin operator along z . Equation (4) actually reflects the fact that the equation of continuity (and hence in our case the dynamic behavior of the center-of-mass coordinate) is deeply influenced by the coupling with the spin variable. The above commutation rule will be later used to exploit the importance of such a coupling in the evaluation of the $m_{-3}(X)$ sum rule.

Another important sum rule is the inverse energy-weighted sum rule, also called dipole polarizability. In the presence of harmonic trapping this sum rule can be calculated in a straightforward way using the commutation relation $[H, P_x] = i\omega_x^2 X$ and the closure relation. One then finds the result $m_{-1}(X) = N/(2\omega_x^2)$, thereby showing that both the energy-weighted and the inverse energy-weighted sum rules relative to the dipole operator X are insensitive to the presence of the spin terms in the single-particle Hamiltonian (2), as well as to the two-body interaction. This does not mean, however, that the dipole dynamic structure factor is not affected by the spin-orbit coupling. This effect is accounted for by another sum rule, particularly sensitive to the low energy region of the excitation spectrum: the inverse cubic energy-weighted sum rule for which we find the exact result

$$m_{-3}(X) = \frac{N}{2\omega_x^4} (1 + k_0^2 \chi) \quad (5)$$

where we have introduced the spin polarizability per particle $\chi = 2m_{-1}(\Sigma_z)/N$ relative to the z -th direction of

the spin operator. In order to derive result (5) we have used the recurrence relation $m_{-3}(X) = m_{-1}(P_x)/\omega_x^4$ following from the commutation relation for $[H, P_x]$, as well as the most relevant commutation rule (4) for $[H, X]$. It is worth mentioning that the above results for the sum rules $m_1(X)$, $m_{-1}(X)$ and $m_{-3}(X)$ hold exactly for the Hamiltonian (1), including the interaction terms. Their validity is not restricted to the mean-field approximation and is ensured for both Bose and Fermi statistics, at zero as well as at finite temperature. In particular the sum rule $m_{-3}(X)$, being sensitive to the magnetic susceptibility, is expected to exhibit a non trivial temperature dependence across the BEC transition.

Equation (5) exploits the crucial role played by the spin-orbit coupling proportional to k_0 . The effect is particularly important when the spin polarizability takes a large value. A large increase of χ is associated with the occurrence of a dipole soft mode as can be inferred by taking the ratio between the inverse and cubic inverse energy-weighted sum rules $m_{-1}(X)$ and $m_{-3}(X)$, yielding the rigorous upper bound $\omega_x/\sqrt{1 + k_0^2 \chi}$ to the lowest dipole excitation energy. The effect of the coupling between the center-of-mass oscillation and the spin degree of freedom is further revealed by making the ansatz $F = P_x + \eta k_0 \Sigma_z$ for the optimized operator exciting the dipole oscillation and minimizing the collective frequency fixed by the ratio

$$\omega^2 = \frac{m_1(F)}{m_{-1}(F)} = \frac{-2\eta^2 k_0^2 \Omega \langle \sigma_x \rangle + \omega_x^2}{1 + (1 + \eta)^2 k_0^2 \chi} \quad (6)$$

with respect to variations of the real parameter η . In deriving the last equality we have explicitly used the sum rule result $m_1(\Sigma_z) = (1/2)\langle 0|[\Sigma_z, [H, \Sigma_z]]|0\rangle = -N\Omega \langle \sigma_x \rangle$ for the energy-weighted moment relative to the spin excitation operator Σ_z . The choice $\eta = 0$ in Eq. (6) corresponds to the estimate $m_{-1}(X)/m_{-3}(X)$. In the opposite $\eta \gg 1$ limit Eq. (6) instead coincides with $m_1(\Sigma_z)/m_{-1}(\Sigma_z)$. Result (6), based on the linear response formalism of sum rules, provides a rigorous upper bound to the dipole frequency in the regime of small amplitude oscillations.

Let us now discuss the behavior of the physical quantities χ and $\langle \sigma_x \rangle$ entering the expression for the dipole frequency. Their actual behavior depends on the quantum phase characterizing the ground state of the many-body system. These phases were investigated in details in [19] for a spin 1/2 interacting Bose-Einstein condensate employing the ansatz

$$\psi = \sqrt{\frac{N}{V}} \left[C_+ \begin{pmatrix} \cos \theta_+ \\ -\sin \theta_+ \end{pmatrix} e^{ik_+ x} + C_- \begin{pmatrix} \sin \theta_- \\ -\cos \theta_- \end{pmatrix} e^{ik_- x} \right] \quad (7)$$

for the order parameter. The variational calculation, applied to a uniform configuration, yields the conditions $k_{\pm} = \pm k_1$ and $\theta_{\pm} = \theta = \arccos(k_1/k_0)/2$ and predicts the occurrence of three quantum phases, depending on the value of the relevant parameters k_0 , Ω and $g_{\alpha\beta}$ (here and in the following we consider a spin symmetric Hamiltonian with $g_{\uparrow\uparrow} = g_{\downarrow\downarrow} = g$ and $\delta = 0$). These are the stripe

¹At finite temperature, the moments m_k should include the proper Boltzmann factors [34]

phase (also called phase I) where Bose-Einstein condensation takes place in a combination of plane waves with opposite momenta $\pm k_1$, provided $g > g_{\uparrow\downarrow}$, the spin-polarized phase II and the single minimum ($k_1 = 0$) phase III. A natural generalization of the variational wave function can be also used to calculate the dynamic properties of uniform matter, by solving the Bogoliubov equations and determining the relevant elementary excitations of the system, the momentum distribution and the quantum depletion of the condensate [35].

The static spin polarizability of the spinor Bose-Einstein condensate at zero temperature can be directly calculated by expanding the values of k_{\pm} and θ_{\pm} around the equilibrium values and minimizing the energy of the system in the presence of an external static field proportional to σ_z . For densities smaller than the critical value $n^{(c)} = k_0^2/(2\gamma g)$, with $\gamma = (g - g_{\uparrow\downarrow})/(g + g_{\uparrow\downarrow})$, all the three phases discussed above are available [19]. In the stripe phase, holding for small Raman frequency Ω , one finds the result

$$\chi_I(\Omega) = \frac{\Omega^2 - 4k_0^4}{(G_1 + 2G_2)\Omega^2 - 8G_2k_0^4}, \quad (8)$$

where we have defined $G_1 = n(g + g_{\uparrow\downarrow})/4$ and $G_2 = n(g - g_{\uparrow\downarrow})/4$ and, for simplicity, we have considered the weak coupling limit characterized by the condition $G_1, G_2 \ll k_0^2$. The spin polarizability χ_I diverges as one approaches the critical frequency $\Omega^{(I-II)} = 2k_0^2\sqrt{2\gamma/(1+2\gamma)}$ providing the transition to the spin-polarized phase. However Eq. (8) is valid only in the low-density limit and inclusion of higher-order terms makes the value of χ finite at the transition. In the spin-polarized phase II the spin polarizability is given by

$$\chi_{II}(\Omega) = \frac{\Omega^2}{(k_0^2 - 2G_2) \left[4(k_0^2 - 2G_2)^2 - \Omega^2 \right]}. \quad (9)$$

It takes a larger and larger value as one approaches the transition point to the zero momentum phase III occurring at the frequency $\Omega^{(II-III)} = 2(k_0^2 - 2G_2)$. In the zero momentum phase III the spin polarizability takes instead the value

$$\chi_{III}(\Omega) = \frac{2}{\Omega - 2(k_0^2 - 2G_2)} \quad (10)$$

exhibiting a divergent behavior when one approaches the transition point from above and vanishing in the limit of large Ω . Results (9) and (10), whose validity is not limited to the weak coupling regime, explicitly reveal the second order nature of the phase transition, the values of χ differing by a factor 2 when one approaches the transition from above or below. They also show that the relevant interaction parameter in both phases is the spin density dependent parameter G_2 . The behavior of the spin polarizability as a function of the Raman coupling Ω is shown in Fig.1 (a) for a choice of parameters which emphasizes the deviations with respect to the weak coupling result. In particular the transition point between the phases II and

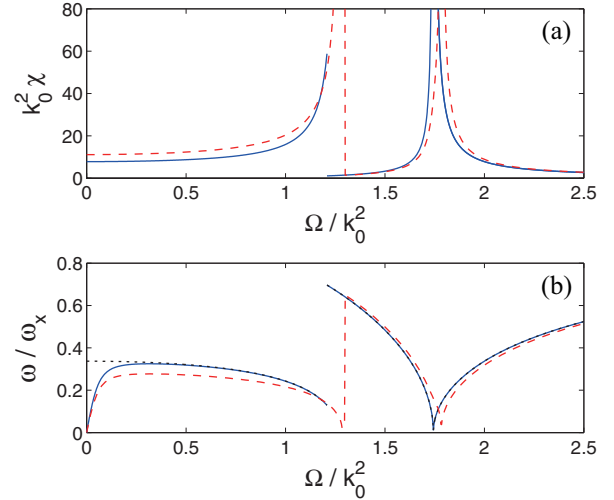


Fig. 1: (Color online) (a) Spin polarizability χ as a function of Ω calculated in uniform matter (blue solid lines) and in the harmonic trap (red dashed lines). (b) The corresponding lowest mode frequency ω with $\langle \sigma_x \rangle$ and χ calculated in uniform matter (blue solid lines) and in the harmonic trap (red dashed lines). The black dotted lines correspond to the prediction $\omega_x/\sqrt{1+k_0^2\chi}$ (see text). The parameters: $k_0^2 = 2\pi \times 320$ Hz, $\omega_x = 2\pi \times 20$ Hz, density in the center of the trap $n \simeq 2.6 \times 10^{13}$ cm $^{-3}$, scattering length $a_{\uparrow\uparrow} = a_{\downarrow\downarrow} = 100 a_B$, $a_{\uparrow\downarrow} = 60 a_B$, where a_B is Bohr radius, corresponding to $G_1/k_0^2 \simeq 0.257$ and $G_2/k_0^2 \simeq 0.064$.

III is predicted to be located at a value $\sim 15\%$ smaller than the value $2k_0^2$ (the weak coupling result). In the same figure we report the value of the spin polarizability calculated within Gross-Pitaevskii theory in the presence of 1D harmonic trapping [19]. The comparison with the uniform matter prediction, corresponding to the value of the density calculated in the center of the trap, is rather good reflecting the usefulness of the uniform matter calculation of χ .

The behavior of the average transverse spin polarization $\langle \sigma_x \rangle$ was calculated in [19]. In the stripe and in the spin-polarized phase the uniform matter calculation yields, respectively, $\langle \sigma_x \rangle = (\Omega/2)/(k_0^2 + G_1)$ and $\langle \sigma_x \rangle = (\Omega/2)/(k_0^2 - 2G_2)$, while in the single minimum phase one has $\langle \sigma_x \rangle = -1$.

We are now in a position to estimate the dipole frequency by minimizing Eq. (6) with respect to the parameter η . The variational procedure actually provides two solutions. The upper solution is physically meaningful only for very small values of Ω where it approaches the frequency ω_x of the center-of-mass sloshing mode. For higher Ω the upper solution takes large values and the coupling with other modes, not accounted for by our ansatz for the excitation operator F , becomes important. The results for the lowest dipole solution are reported in Fig.1 (b). They reveal the important deviations from the oscillation frequency ω_x caused by the spin-orbit and Raman couplings for all values of Ω . In the same figure we also show

the prediction $\omega_x/\sqrt{1+k_0^2\chi}$ for the dipole frequency, obtained by setting $\eta = 0$ in (6). This turns out to be an excellent estimate except for very small values of the Raman coupling. Actually, in the $\Omega \ll \omega_x$ limit the value of η minimizing Eq. (6) is no longer small and the mode turns out to be a pure spin oscillation, its frequency vanishing linearly with Ω . In this limit the mode does not exhibit any significant coupling with the center-of-mass oscillation. At the transition between the phases I and II the lowest dipole frequency exhibits a sudden jump and then starts decreasing for larger values of Ω . In the thermodynamic limit, it vanishes at the transition between the phases II and III as a consequence of the divergent behavior of χ and, above the transition, it increases to reach asymptotically the oscillator value ω_x at large Ω .

In Fig.2 we show the spin polarizability and the frequency of the lowest dipole mode calculated in the experimental conditions of [8]. They correspond to a very small value of γ ($\sim 10^{-3}$), thereby causing the compression of the stripe phase into a narrow region at small values of Ω . Furthermore these conditions correspond to a very small value of G_2 . As a consequence, in the wide range of Raman coupling $\Omega \gg \omega_x$ Eqs. (6), (9) and (10) yield the useful results

$$\omega_{\text{II}}^2 = \omega_x^2 (1 - \Omega^2/4k_0^4), \quad \omega_{\text{III}}^2 = \omega_x^2 (1 - 2k_0^2/\Omega) \quad (11)$$

for the dipole frequency in the phases II and III. Fig.2 (a) shows in a clear way the divergent behavior of the spin polarizability at the transition between the two phases which is responsible for the quenching of the dipole frequency. The GP simulations are practically indistinguishable from the calculations of χ in the uniform matter (and hence of ω) based on uniform matter ingredients. The comparison with the experimental data for the dipole frequencies, as shown in Fig.2 (b), is good far from the transition point at $\Omega = 2k_0^2$, while near the transition nonlinear effects play a major role as discussed in [8] (see also discussion below).

The combined spin-orbit nature of the lowest dipole mode is also nicely revealed by the relative amplitudes of the oscillating values of the center-of-mass position (A_X), momentum (A_P) and spin polarization (A_Σ). These amplitudes can be calculated in the present approach by writing the many body oscillating wave function as $|\psi(t)\rangle = e^{i\alpha(t)F} e^{\beta(t)D}|0\rangle$ where $F = P_x + \eta k_0 \Sigma_z$ is the excitation operator and D is defined by the commutation relation $[H, D] = F$, while α and β are parameters whose time dependence can be obtained through a variational Lagrange procedure. The time dependence of the relevant quantities $\langle X \rangle$, $\langle P_x \rangle$ and $\langle \Sigma_z \rangle$ is then easily calculated by expanding the wave function up to first order in α and β . For $\Omega \ll \omega_x$, as discussed above, the lowest frequency mode is mainly a spin oscillation (large η) and one finds that the center-of-mass position is basically at rest ($A_X \sim 0$), while $A_P/k_0 \sim A_\Sigma$. For larger values of Ω the lowest frequency is instead well approximated by the choice $\eta = 0$, and the relationships

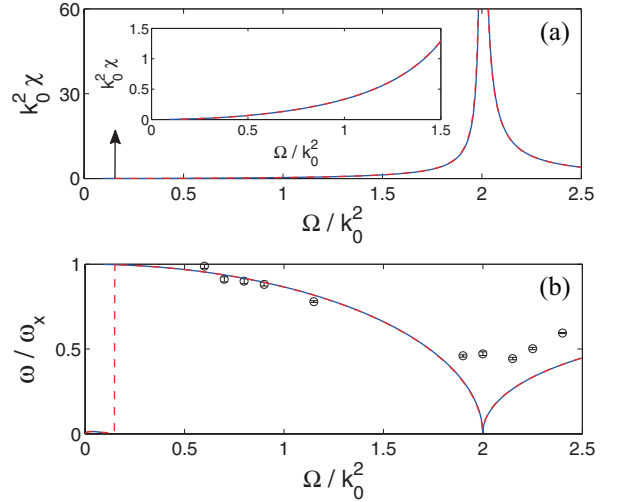


Fig. 2: (Color online) (a) Spin polarizability χ and (b) lowest mode frequency ω as functions of Ω (see Fig.1 for details) with different choice of parameters: $k_0^2 = 2\pi \times 4.42$ kHz, $\omega_x = 2\pi \times 45$ Hz, density in the center of the trap $n \simeq 1.37 \times 10^{14} \text{ cm}^{-3}$, scattering length $a_{\uparrow\uparrow} = a_{\downarrow\downarrow} = 101.20 a_B$, $a_{\uparrow\downarrow} = 100.99 a_B$, where a_B is Bohr radius, and the atomic mass of ^{87}Rb . The black circles are the experimental data of [8]. The black arrow in (a) indicates the transition between the phase I and II.

between the spin, center-of-mass and momentum amplitudes take the useful form $A_\Sigma = A_X k_0 \omega_x \chi / \sqrt{1+k_0^2\chi}$ and $A_P/k_0 = A_\Sigma (1+k_0^2\chi) / (k_0^2\chi)$. The connection between the momentum and spin amplitudes has been already pointed out in [8]. The above relationships show that, near the transition between the phases II and III, where the spin polarizability diverges, the amplitude A_Σ of the spin oscillation can easily take large values, thereby emphasizing the role of nonlinear effects. These effects are likely at the origin of the finite values of the dipole frequencies observed at the transition (see Fig. 2 and discussion in [8]). It is finally worth mentioning that, despite its strong spin nature, the lowest frequency mode exhausts almost completely the dipole polarizability sum rule $m_{-1}(X)$, except in the $\Omega \ll \omega_x$ region. As a consequence it can be easily excited by displacing the trapping potential.

In the last part of the work we show that a useful insight on the lowest dipole oscillation can be also obtained by investigating the dynamic behavior employing directly the lower branch

$$\epsilon(\mathbf{p}) = \frac{1}{2} (p_x^2 + p_\perp^2 + k_0^2) - \frac{1}{2} \sqrt{4p_x^2 k_0^2 + \Omega^2} \quad (12)$$

of the excitation spectrum of uniform matter. The new single particle Hamiltonian can be used to solve the classical Hamilton-Jacobi equations in both the linear and nonlinear regimes [8]. It can be also used to calculate the ratio $m_1(X)/m_{-1}(X)$ between the energy-weighted and inverse energy-weighted sum rules relative to the dipole operator X . While the result $N/(2\omega_x^2)$ for the dipole polarizability continues to hold, the energy-weighted moment

is deeply affected by the new Hamiltonian reflecting the projection procedure accounted for by Eq. (12). By carrying out explicitly the double commutator one finds the result $\omega^2 = \omega_x^2 \langle \partial_{p_x}^2 \epsilon(\mathbf{p}) \rangle$. By replacing the value of p_x with the value where $\epsilon(\mathbf{p})$ is minimum, i.e., where Bose-Einstein condensation takes place in uniform matter (effective mass approximation), one recovers the results (11) predicted by the sum rule approach in the weak coupling limit in the phases II and III respectively. A better estimate of the frequency at the transition point $\Omega = 2k_0^2$ can be obtained by evaluating the integral $\int d\mathbf{p} n(\mathbf{p}) \partial_{p_x}^2 \epsilon(\mathbf{p})$ with $n(\mathbf{p})$ given by the momentum distribution of the Gross-Pitaevskii solution in the presence of the harmonic trap. With the choice of parameters of Fig.2 we find $\omega_{\min} \simeq 0.03 \omega_x$. The use of lowest branch dispersion (12) turns out to be instead unsuitable to investigate the lowest dipole frequency in the stripe phase.

In conclusion we have developed a sum rule description of the dipole oscillation which explicitly reveals the crucial role played by the spin polarizability in the presence of spin-orbit coupling. The method can be also applied to Fermi gases as well as generalized to study the coupling between the dipole and other collective oscillations recently pointed out in [31].

Note added after submission: the divergent behavior of the magnetic susceptibility predicted in the present work has been recently observed experimentally in [36] through the analysis of the relative spin and momentum amplitudes.

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